Butylamine
109-73-9 | DTXSID1021904

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 10.0 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.26e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

Image not found
Butylamine
Measured: 13.7
Predicted: 10.0

Image not found
Isobutylamine
Measured: 13.7
Predicted: 10.4

Image not found
2-Butanamine
Measured: 1.53
Predicted: 5.31

Image not found
Pentan-1-amine
Measured: 11.5
Predicted: 6.46

Image not found
Propylamine
Measured: 16.9
Predicted: 17.1